4,4'-Methylenedianiline 101-77-9 | DTXSID6022422

Model	Performance
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Model	Data	

Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.84	0.55	0.85	0.53	0.83	0.64	

Model Results

Predicted value: 3.73

Global applicability domain: Inside

Local applicability domain index: 4.87e-01

Confidence level: 6.67e-01

Nearest Neighbors from the Training Set

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2,2,4-Trimethyl-1,3-pentanediol

Measured: 1.00 Predicted: 1.47

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2,2-Bis(bromomethyl)-1,3-

propanediol Measured: 4.79 Predicted: 3.35

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4-IsobutyImorpholine Measured: 1.78 Predicted: 2.69

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Molinate

Measured: 25.7 Predicted: 14.8

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O,O-Diethyl dithiophosphate

Measured: 5.01 Predicted: 5.43